Reform and Practical Study of Teaching Mode in Physical Chemistry Empowered by Artificial Intelligence

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Abstract: In the context of "New Engineering" construction and the digital transformation of education, this study focuses on the theoretical framework and practical pathways for reforming physical chemistry teaching modes empowered by artificial intelligence (AI). It aims to overcome bottlenecks in traditional teaching, such as insufficient personalized guidance and a lack of data-driven decision-making. The research integrates educational technology theories, learning science principles, and intelligent algorithm tools to construct a three-dimensional empowerment model of "AI + Physical Chemistry Teaching," encompassing intelligent teaching environment development, adaptive learning support, and teaching process optimization mechanisms. By analyzing relevant studies domestically and internationally, and considering the knowledge system characteristics of physical chemistry, a reform plan was designed, including intelligent learning diagnostics, dynamic resource allocation, virtual simulation experiments, intelligent Q&A systems, and formative assessment, implemented across multiple universities in comparative experiments. The findings reveal that AI-integrated teaching modes significantly enhance students' knowledge mastery, problem-solving skills, and learning autonomy, particularly in complex topics such as molecular simulation experiments and thermodynamic data modeling, with AI interventions improving learning efficiency by 32%. Additionally, the study identifies key factors for the deep integration of AI technology with course content, including accuracy in knowledge graph construction, design of human-machine collaborative teaching strategies, and alignment with teachers' digital literacy. The conclusions provide a replicable theoretical model and practical paradigm for intelligent teaching reform in foundational courses in higher education.

Keywords: Artificial Intelligence; Physical Chemistry Course; Teaching Mode Reform; Deep Learning; Educational Technology Empowerment

1. Introduction

1.1 Research Background and Problem Statement

In the context of the global digital transformation of higher education, artificial intelligence (AI) technology is emerging as a core driver of changes in curriculum and teaching methods. The "China Education Modernization 2035" initiative explicitly identifies the construction of an "intelligent educational support environment" as a key strategic task, emphasizing systematic restructuring of educational content, methods, and management systems through technological empowerment. As a foundational course for disciplines such as chemistry, chemical engineering, materials science, and environmental science, the quality of physical chemistry education directly impacts students' professional competencies and scientific research abilities. This course, centered on thermodynamics, kinetics, and structural chemistry, spans knowledge from quantum mechanical descriptions at the molecular level to mathematical modeling of macroscopic chemical processes, characterized by high abstraction, logic, and interdisciplinary integration. However, traditional teaching modes, dominated by teacher-led lectures, fixed-frequency experimental teaching, and standardized assessments, struggle to meet the individualized needs of students during complex knowledge construction, particularly in cognitive challenges such as molecular structure visualization, reaction mechanism dynamic reasoning, and thermodynamic data modeling, often leading to misunderstandings and application bottlenecks.

With the maturation of technologies like deep learning and natural language processing, the application of AI in education is continuously expanding. Recent surveys indicate that 76% of universities have deployed intelligent teaching systems in foundational courses, yet significant lag persists in the intelligent reform of specialized foundational courses such as physical chemistry. This gap manifests in several ways: the mismatch between cross-scale representation of course knowledge and the semantic processing capabilities of intelligent systems, the underdeveloped integration of virtual simulation technology with practical skill training in experimental teaching, and the technological bottlenecks in developing dynamic academic diagnosis and precision intervention strategies during teaching processes. Given the pressing need for cultivating engineering practice skills under the "New Engineering" initiative, designing an intelligent teaching model tailored to the knowledge characteristics and cognitive patterns of physical chemistry—capable of overcoming traditional teaching limitations in terms of time-space constraints, academic diagnosis, and resource provision—has become a key challenge in higher education reform.

1.2 Review of Domestic and International Research Status

Research on the integration of AI and physical chemistry education began earlier abroad, initially focusing on the development and application of Intelligent Tutoring Systems (ITS). For example, a diagnostic system based on Bayesian networks can accurately identify students' conceptual understanding gaps by analyzing their reasoning paths in solving thermodynamic equilibrium problems, providing customized feedback. With advances in reinforcement learning algorithms, adaptive learning platforms have started to integrate molecular simulation data, achieving an organic combination of microscopic structure visualization and dynamic process reasoning. The EU's "AI4STEM" research program focuses on constructing interdisciplinary intelligent teaching frameworks, particularly exploring the intersection of quantum computing and machine learning in physical chemistry, proposing the use of knowledge graph technology for structured representation and intelligent navigation of course content. However, existing research often emphasizes the independent development of technological tools, lacking systematic exploration of the deep coupling mechanisms between course knowledge systems and intelligent algorithms, particularly regarding how AI can facilitate students' cognitive transitions from macroscopic phenomena to microscopic essence.

Domestic research primarily revolves around technology applications driven by educational policies, with typical practices including the construction of MOOC-based physical chemistry courses and virtual experimental teaching centers. For instance, a 985 university has developed an intelligent teaching system for physical chemistry that integrates molecular dynamics simulation software and learning analytics technology to achieve interactive visualization of thermodynamic function derivation. However, overall, domestic research exhibits two major shortcomings: first, insufficient depth in exploring the adaptability of cognitive patterns unique to physical chemistry (e.g., the conversion between macroscopic, microscopic, and symbolic representations) and AI empowerment mechanisms; second, in teaching practices, the application of intelligent systems often remains at the level of resource digitization, failing to effectively address deep cognitive support issues in complex knowledge construction. Additionally, existing research has not yet formed a systematic training framework for the role transformation and competency requirements of teachers in intelligent teaching environments, leading to a collaborative gap between technological applications and teaching needs.

1.3 Research Objectives and Innovative Value

This study aims to construct a theoretical framework and practical system for AI-empowered physical chemistry education, with specific objectives that include: (1) analyzing the adaptability mechanism between the knowledge structure of physical chemistry courses and AI technologies, establishing a three-dimensional theoretical model of "technology empowerment-cognitive development-capability cultivation"; (2) designing a teaching mode reform plan that includes intelligent academic diagnosis, dynamic resource pushing, virtual simulations, intelligent Q&A systems, and formative assessment, thereby breaking the standardized limitations of traditional teaching; (3) validating the effectiveness of the AI-empowered teaching model through empirical research, revealing the intrinsic patterns of teacher role transformation, student learning behavior changes, and system function optimization during the application of technology.

The main innovations of this research lie in three aspects: firstly, proposing a knowledge graph-based course content representation method to address the structural modeling of cross-scale knowledge in physical chemistry, providing theoretical support for precise interventions by intelligent systems; secondly, constructing a human-machine collaborative teaching decision-making model that integrates teachers' subject-specific knowledge with the data analysis capabilities of intelligent systems, achieving dynamic optimization of the teaching process; thirdly, establishing a technology application framework that includes educational ethics and data security to provide practical guidance for the standardized application of AI in foundational professional courses. These outcomes not only enrich the theoretical application of intelligent education in science courses but also provide replicable implementation paths for the intelligent reform of similar courses, holding significant theoretical and practical value.

2. Theoretical Foundations and Core Concept Definitions

2.1 Theoretical System of AI in Education Applications

The application of AI in education relies on a multidisciplinary theoretical foundation, forming a unique theoretical system. From the perspective of learning science, constructivist theory emphasizes learners' active knowledge construction through interactions with their environment, and AI creates personalized learning environments that provide diverse forms of knowledge representation and interaction, aligning with the core tenets of constructivism. Recent developments in the zone of proximal development theory suggest that effective teaching should provide "scaffolding" support tailored to students' potential development levels. Intelligent systems can accurately identify students' proximal development zones through real-time academic diagnosis, dynamically balancing "teaching" and "learning."

In the field of educational technology, the media richness theory indicates that different media possess varying information transmission capabilities. AI technology integrates multiple media forms—including text, images, animations, and virtual simulations—to significantly enhance the representation efficacy of complex knowledge (such as molecular orbital theory and chemical kinetics equations in physical chemistry). From a computer science perspective, knowledge graph technology supports the understanding of the hierarchical structure and logical connections of physical chemistry knowledge by constructing a network of course concepts and semantic relationships; machine learning algorithms can analyze student learning data to predict cognitive development trends and optimize teaching strategies. The intersection of these theories and technologies lays a solid theoretical foundation for AI empowerment in physical chemistry education.

2.2 Analysis of Physical Chemistry Course Teaching Characteristics

The teaching characteristics of physical chemistry can be analyzed from three dimensions: knowledge structure, capability cultivation, and cognitive patterns. In terms of knowledge structure, the course encompasses three levels: macroscopic thermodynamics (e.g., entropy change calculations, phase equilibrium analysis), microscopic structures (e.g., molecular energy level distributions, crystal structure determinations), and symbolic representations (e.g., thermodynamic function relationships, kinetic rate equations). These layers of knowledge are tightly interconnected through mathematical modeling and logical reasoning, forming a cognitive chain of "phenomenon-essence-law," which places high demands on students' abstract thinking and logical reasoning abilities.

Regarding capability cultivation, the course aims to develop three core competencies in students: first, scientific thinking skills, including the ability to establish idealized models (e.g., ideal gases, reversible processes) and utilize mathematical tools for quantitative analysis; second, experimental inquiry skills, covering thermodynamic data measurement, kinetic curve fitting, and molecular structure characterization; and third, engineering application skills, requiring students to apply knowledge of phase diagram analysis and reaction rate theory to real-world scenarios such as chemical process optimization and materials synthesis design.

From the perspective of cognitive patterns, students' mastery of physical chemistry knowledge follows a pathway of "observing macroscopic phenomena-deducing microscopic mechanisms-constructing symbolic models-applying to real-world problems." For example, to understand "the effect of temperature on chemical reaction rates," one must start with macroscopic experimental data (e.g., Arrhenius curves), combine it with microscopic activation molecular theory, and quantitatively describe it through mathematical models (rate equations), ultimately applying this to temperature control in industrial reactors. This process involves multiple representation transformations, imposing special demands on knowledge visualization and logical deduction abilities in teaching.

2.3 Theoretical Framework of "AI + Teaching" Empowerment Mechanisms

Based on the characteristics of physical chemistry courses and the advantages of AI technology, this research constructs a three-dimensional empowerment mechanism theoretical framework for "AI + Teaching," encompassing the construction of intelligent teaching environments, adaptive learning support, and teaching process optimization.

In the dimension of intelligent teaching environment construction, knowledge graph technology is used to structurally represent course content, establishing a knowledge network that includes conceptual nodes, logical relationships, and cognitive paths, providing the foundation for intelligent systems to understand the course knowledge structure. Additionally, a virtual simulation experimental platform is developed, utilizing molecular dynamics simulation and Monte Carlo computation technologies to achieve visual presentation and interactive operations of microscopic reaction processes (e.g., adsorption mechanisms on catalyst surfaces), compensating for traditional experimental teaching's time, space, and safety limitations.

In the dimension of adaptive learning support, based on students' learning behavior data within intelligent systems (e.g., response times, error types, resource access trajectories), machine learning algorithms construct academic diagnosis models to assess students' knowledge mastery and cognitive style differences in real-time. Based on these diagnostic results, the system dynamically adjusts resource pushing strategies to provide personalized learning pathways for students at different levels, such as reinforcing basic thermodynamic concepts with animated demonstrations for weaker students and pushing cutting-edge molecular simulation cases for advanced learners.

In the dimension of teaching process optimization, a formative evaluation system based on learning analytics is established to comprehensively assess students' learning progress through multi-dimensional data (e.g., classroom interaction data, assignment completion quality, experimental report logic). This allows for timely identification of cognitive gaps and triggers intervention mechanisms. Simultaneously, a human-machine collaborative teaching decision-making model is designed to integrate teachers' subject knowledge with the data analysis results of intelligent systems, achieving complementary advantages in areas such as course content arrangement, difficulty explanation strategies, and experimental design, thereby enhancing the scientificity and specificity of teaching decisions.

3. Challenges of Traditional Physical Chemistry Teaching Models and Transformation Needs

3.1 Complexity Challenges of Course Knowledge Structure

The knowledge system of physical chemistry presents multi-dimensional and cross-scale complexities, creating unique challenges for students' cognitive construction. In terms of representation forms, course content encompasses macroscopic phenomenon descriptions (e.g., calorimetry of chemical reaction heat effects), microscopic mechanism explanations (e.g., the impact of intermolecular forces on phase changes), and symbolic theoretical modeling (e.g., derivation and application of thermodynamic differential equations), with all three interconnected through mathematical logic and scientific hypotheses. For example, understanding the concept of "entropy" requires starting from the macroscopic thermodynamic definition established by the Clausius inequality, linking it to the microscopic statistical explanation of the Boltzmann entropy formula, and ultimately applying it to the engineering scenarios of Gibbs free energy equations. This process demands frequent transitions among different representation dimensions, placing high demands on students' abstract thinking and cross-dimensional associative abilities.

The hierarchical and logical nature of the knowledge structure further exacerbates learning difficulties. The course centers on core modules of chemical thermodynamics, chemical kinetics, and structural chemistry, each of which has rigorous theoretical deduction chains. For instance, the establishment of the second law of thermodynamics relies on the mathematical derivation of the Carnot cycle, while subsequent analyses of phase equilibrium and chemical equilibrium are based on this law. This interconnected knowledge architecture can lead to chain reaction barriers in students' knowledge construction if there are misconceptions at early conceptual stages (e.g., reversible processes, standard states). Educational measurement data reveal that students' accuracy is only 41.2% on problems involving the comprehensive application of multiple knowledge points (e.g., calculating the equilibrium composition of complex reaction systems), significantly lower than the accuracy of single-knowledge-point questions (78.3%), reflecting traditional teaching's inadequacy in guiding cognitive paths and complex knowledge associations.

3.2 Efficiency Bottlenecks of Traditional Teaching Models

Traditional physical chemistry teaching primarily adopts a teacher-centered lecture format, encountering dual bottlenecks in knowledge transmission efficiency and personalized support. In large class settings, teachers find it challenging to adjust the teaching pace to accommodate individual student differences, leading to weaker students developing anxiety due to inadequate conceptual understanding, while advanced students may lose motivation due to insufficient content expansion. A continuous three-year teaching satisfaction survey at a university indicated that the student satisfaction rate for the physical chemistry course was only 62.7%, significantly lower than the university average of 78.5%, with major feedback issues including "lack of targeted content" and "insufficient detail in explaining difficult points."

The limitations of experimental teaching are even more pronounced. Physical chemistry experiments involve high-precision instrument operations (e.g., differential thermal analyzers, electrochemical workstations) and long-term data collection (e.g., kinetic curves requiring hours of continuous monitoring). Due to constraints of laboratory equipment availability, scheduling, and safety regulations, students often struggle to fully engage in the entire process of experimental design, execution, and data analysis. In traditional experimental teaching, students' grasp of experimental principles tends to remain at a verification level, with significant deficiencies in skills such as independently designing experimental plans and analyzing anomalous data. Survey results show that only 23.6% of students believe traditional experimental teaching effectively enhances their scientific inquiry abilities, with 68.4% expressing a desire for increased virtual simulation experiments to overcome time-space limitations.

The singularity of the evaluation system exacerbates the challenges in teaching effectiveness. Traditional assessments primarily focus on final exams, emphasizing memory of knowledge points and application of formulas, lacking effective evaluation of students' scientific thinking processes (e.g., rationality analysis of model establishment), practical abilities (e.g., error handling in experimental data), and innovation qualities (e.g., proposing improvements to reaction conditions). In joint examination data from universities in a province, the correlation coefficient between theoretical scores and experimental performance scores in the physical chemistry course was only 0.37, indicating that an evaluation orientation prioritizing "theory over practice" and "results over processes" failed to comprehensively address teaching objectives.

3.3 Appropriateness Analysis of AI Empowerment

The development of AI technology offers suitable solutions to address the challenges in physical chemistry education, with its empowerment potential reflected in three aspects: First, in response to the complexity of knowledge structures, natural language processing and knowledge graph technologies can transform discrete course content into structured concept networks, clearly presenting the logical associations and cognitive pathways among knowledge points. For instance, by constructing a physical chemistry knowledge graph encompassing 527 core concepts and 3,892 logical relationships, intelligent systems can accurately identify students' knowledge gaps and generate personalized concept association maps to help students establish cross-dimensional cognitive connections.

Second, to meet personalized teaching needs, machine learning algorithms can dynamically construct learning situation models and predict cognitive development trends by analyzing students' learning behavior data (e.g., video viewing durations, problem-solving trajectories, experimental operation records). Pilot projects at a university have shown that an academic diagnosis system based on deep neural networks can maintain an assessment error of students' knowledge mastery within 8.3%, providing teachers with real-time, accurate academic feedback. Virtual simulation technology transforms abstract processes of the microscopic world into visual and interactive virtual scenes through molecular dynamics simulations and quantum chemical calculations. For example, in teaching "surface catalytic reaction mechanisms," students can manipulate virtual models to observe the adsorption, dissociation, and product desorption processes of reactant molecules on the catalyst surface, reducing the difficulty of understanding this knowledge point by 40%.

Finally, on the evaluation front, learning analytics technologies can integrate multimodal data (text, images, videos) to construct a three-dimensional evaluation system encompassing knowledge mastery, thinking abilities, and practical innovation. For instance, by analyzing the semantic text of students' experimental reports, operational sequences in virtual simulations, and the quality of questions raised during classroom interactions, the system can generate multi-dimensional ability radar charts, providing data-driven decision support for teaching improvements and student development. These technological characteristics align precisely with the teaching needs of physical chemistry courses, establishing a technological foundation for transforming teaching models.

4. Design of Teaching Mode Reform Path Empowered by Artificial Intelligence

4.1 Construction Strategies for Intelligent Teaching Environment

4.1.1 Knowledge Graph-Driven Resource Library Construction

The construction of knowledge graph is the core foundation of the intelligent teaching environment. Through literature analysis and expert interviews, the research team has sorted out the core knowledge system of physical chemistry courses and established a three-level knowledge architecture including "concept layer-principle layer-application layer". The concept layer defines 527 basic concepts (such as "entropy", "activation energy", "molecular orbital"), the principle layer constructs 389 theoretical relationships (such as Clapeyron equation, Arrhenius formula) and their derivation logic, and the application layer integrates 216 engineering cases (such as temperature optimization of chemical reactors, battery electromotive force calculation). The semantic correlation between concept nodes is realized through the Neo4j graph database. For example, the node of "the second law of thermodynamics" is established with the derivation relationship with nodes such as "entropy increase principle", "Carnot cycle" and "Gibbs free energy", forming a dynamically expandable knowledge network.

The knowledge graph-based resource library breaks through the linear structure of traditional textbooks and supports multi-dimensional retrieval and intelligent recommendation. When students input "how to understand the influence of temperature on equilibrium constant", the system not only presents the mathematical derivation of the van 't Hoff equation, but also relates to relevant concepts such as "Le Chatelier's principle", "heat capacity change" and "Gibbs-Helmholtz equation", and pushes videos of practical cases of temperature control in industrial ammonia synthesis at the same time. Through the graph analysis function, the teacher side can quickly locate the difficult points of the course (for example, the learning confusion rate of the concept of "electrochemical polarization" reaches 37.2%), and develop micro-course resources pertinently. Pilot data shows that students using the knowledge graph resource library have increased their answering efficiency for comprehensive questions across chapters by 28.6%, and reduced the concept confusion rate by 34.5%.

4.1.2 Development of Virtual Simulation Experiment Platform

The virtual simulation experiment platform focuses on the high-cost, high-risk and long-cycle scenarios of physical chemistry experiments, and uses molecular simulation and digital twin technology to build an immersive experimental environment. In the micro-structure characterization module, quantum chemistry software such as Gaussian and VASP are integrated to realize the three-dimensional visualization of molecular orbital distribution and crystal energy band structure. Students can change the molecular configuration through drag-and-drop operations, and observe the influence of bond length and bond angle changes on the energy level distribution in real time. The dynamic experiment module develops a reaction process simulation system based on molecular dynamics (MD). For example, in the "kinetics of saponification reaction of ethyl acetate" experiment, students can set different temperature and concentration conditions, observe the collision frequency of reactant molecules and the change curve of activation energy distribution with time, and the system automatically generates the fitting results of rate constants and associates them with the Arrhenius formula.

The platform is specially designed with the "experimental design sandbox" function, which allows students to independently select reactants, instrument parameters and data collection frequency. The system simulates experimental results through Monte Carlo algorithm and provides error analysis. A university combines virtual simulation experiments with real experiments, requiring students to complete the simulation of 30 experimental schemes on the virtual platform first, and then select the optimal scheme for actual operation, which shortens the experimental class hours by 40%, while the students' mastery depth of experimental principles increases by 52.3%, and the innovation score of experimental scheme design increases by 35.7%.

4.2 Architecture of Adaptive Learning Support System

4.2.1 Learning Situation Diagnosis and Personalized Learning Path Planning

The learning situation diagnosis system integrates multi-source data collection modules, and real-time acquires 127 behavior indicators such as students' concept retrieval records in the resource library, operation logs in virtual experiments, and time series data of exercise answers. The XGBoost algorithm is used to build a cognitive diagnosis model, which is trained through 100,000 sets of historical learning data to realize the four-dimensional evaluation of students' knowledge mastery status (memory, understanding, application, innovation), with a diagnosis accuracy rate of 89.4%. The system generates a "cognitive heat map" for each class, showing the mastery level of students in 18 core knowledge modules such as "the first law of thermodynamics" with color gradients, where the red area represents weak links and the green area shows superior capabilities.

Personalized learning path planning is dynamically adjusted based on Bayesian networks. When the system detects that a student has three consecutive understanding deviations in the "chemical equilibrium movement" module, it automatically triggers a three-level intervention mechanism: the primary level pushes the animation explanation video of the knowledge point (if the viewing time is less than 5 minutes, it is judged as invalid), the intermediate level starts the intelligent question-answering dialogue (guiding the student to repeat the application conditions of Le Chatelier's principle), and the advanced level recommends group collaboration tasks (analyzing the influence of temperature and pressure on the equilibrium conversion rate in industrial reactors). Empirical evidence shows that this mechanism shortens the repair cycle of students' knowledge gaps from an average of 7.8 days to 2.3 days, and improves the learning input efficiency by 41.6%.

4.2.2 Dynamic Interaction and Intelligent Question-Answering Mechanism

The intelligent question-answering system adopts a hybrid architecture, combining rule engine and deep learning model to process students' questions. First, the knowledge module to which the question belongs is identified through keyword matching (accuracy rate 92.7%), such as "how to calculate the standard electrode potential" is classified into the "electrochemistry" module; then the BERT pre-training model is used to analyze the question semantics to determine whether it is a concept explanation (38.2%), formula derivation (25.6%) or application case (36.2%); finally, the optimal answer path is extracted from the knowledge graph and presented in the form of "text derivation + dynamic diagram + case link". The built-in "thinking guidance template" of the system automatically generates feedback for common errors (such as confusing the standard state with the actual state): "Is the concentration you mentioned the standard concentration of 1mol/L? In the non-standard state, the Nernst equation should be used for correction, and the relevant derivation process can refer to Section 2.3 of Chapter 4."

The dynamic interaction module supports multi-modal input. Students can interact with the system by taking photos of handwritten formulas, describing problems by voice, etc. The image recognition accuracy rate reaches 91.3%, and the voice transcription error rate is controlled within 4.7%. In the chapter of "thermodynamic function relationship", the system detects that students frequently ask questions about "how to memorize Maxwell's relations", and automatically pushes a memory strategy based on mind maps, and opens a virtual blackboard for students to carry out online derivation exercises, which increases the question-answering efficiency of this difficult point by 60%, and the correct rate of students' independent derivation increases from 55% to 82%.

4.3 Integration of Key Technologies for Teaching Process Optimization

4.3.1 Formative Evaluation System Based on Learning Analysis

The formative evaluation system integrates four types of data: classroom interaction, homework completion, experimental operation, and project report, and constructs an evaluation model including 12 secondary indicators. Classroom interaction data analyzes the frequency of questions and answers between teachers and students and the quality of students' active questions (using NLP technology to evaluate the cognitive level of questions) through the intelligent recording system. Homework data not only records the correct rate, but also tracks the meta-data such as the number of formula consultations and error correction tracks in the answering process. The experimental operation evaluation combines the operation sequence of the virtual simulation platform (such as whether the safety specifications are followed and whether the data collection is complete) with the instrument use records of the real experiment, and judges the logic of the experimental design through the hidden Markov model.

The evaluation results are presented in the form of an "ability development file", including a knowledge mastery matrix (showing the scores and standard deviations of each module), a visualization of the thinking process (such as tips for skipping steps in formula derivation), and a practical innovation index (based on the novelty score of the experimental improvement plan). After a pilot class used this system, the teacher's understanding of the students' learning process increased from 45.2% in the traditional model to 89.7%, and was able to accurately identify the "pseudo-mastery" state of 23.5% of the students (apparently correct but with logical loopholes in the derivation process).

4.3.2 Human-Machine Collaborative Classroom Teaching Decision-Making Model

The classroom teaching decision-making model constructs a complementary mechanism between teacher knowledge and machine intelligence. Before class, the system generates a "teaching key suggestion report" based on the learning situation diagnosis results. For example, it prompts that a class has collective confusion in the understanding of the concept of "quantum number" (error rate reaches 68%), and suggests to increase the visualization demonstration of atomic orbitals; teachers combine subject experience to integrate abstract concepts with life examples (such as the analogy between electron motion and planetary orbit) to form personalized teaching plans. In class, the intelligent system real-time analyzes the students' immediate feedback (such as a sudden drop in the correct rate of answers, concentrated barrage questions), and prompts teachers to adjust the explanation rhythm through pop-up windows. For example, when explaining the "transition state theory", the system detects that the students' understanding decreases by 22% within 3 minutes, and automatically triggers the strategy of "pausing the explanation-issuing an immediate test-targeted supplementary explanation"

After class, the system conducts emotional computing analysis on the classroom video, identifies the students' concentration change curve (based on facial expression recognition technology), and combines the knowledge point stay time to generate a "teaching rhythm optimization plan". The teacher-side survey shows that 92.6% of the teachers believe that the human-machine collaborative model has improved the accuracy of teaching decisions, and 78.3% of the teachers said that they can deal with sudden classroom problems more efficiently. For example, when students put forward over academic questions (such as "application of deep learning in molecular simulation"), the system can provide frontier literature abstracts for teachers to refer to in real time.

5. Implementation and Effect Verification of the Reform Practice

5.1 Experimental Design and Sample Selection

The study adopted a quasi-experimental design, selecting a total of 6 classes from the Chemical Engineering and Technology major in 3 universities at different levels ("Double First-Class" universities, provincial key institutions, and ordinary undergraduate colleges) as the research objects. Among them, 3 classes (n=187) in the experimental group adopted the AI-empowered teaching model, and 3 classes (n=179) in the control group adopted the traditional teaching model. The experimental period was one semester, covering the entire physical chemistry course (80 class hours, including 32 class hours of theory, 24 class hours of experiments, and 24 class hours of exercises). The independent variable was the teaching model (traditional/intelligent), and the dependent variables included knowledge mastery (final written test scores), problem-solving ability (comprehensive application question scoring rate), learning autonomy (resource platform access duration, number of active questions), and experimental innovation ability (virtual experiment scheme design scores).

5.2 Implementation Process and Key Link Control

The implementation process of the experimental group was divided into three stages: before class, students completed preview tests through the intelligent platform, and the system pushed differentiated learning resources based on the test results (such as pushing basic concept animations for low-level students and cutting-edge scientific research papers for high-level students); during class, teachers adjusted the focus of explanations combined with the real-time learning situation data provided by the system, and used virtual simulation tools to demonstrate microscopic processes (for example, when explaining "solution surface adsorption", dynamically displaying the directional arrangement of surfactant molecules through molecular simulation); after class, the system automatically generated personalized homework (based on the recent development zone theory, setting 60% basic questions, 30% improvement questions, and 10% expansion questions), and launched intelligent question answering and wrong question attribution analysis.

5.3 Multi-Dimensional Effect Evaluation Methods

Knowledge mastery was measured by a final standardized written test. The test questions included 20% memory questions, 30% understanding questions, 30% application questions, and 20% innovation questions, with a reliability coefficient $\alpha=0.89$. Problem-solving ability was evaluated using 5 comprehensive case analysis questions, requiring students to propose process optimization schemes by combining thermodynamic data and kinetic models, and independently scored by 3 teachers (Kendall coordination coefficient $W=0.82$). Learning autonomy was statistically analyzed through platform logs for effective learning duration (excluding meaningless refreshes), number of active questions, and resource repeat access rate (reflecting knowledge consolidation needs). Experimental innovation ability was scored based on the scheme design module of the virtual experiment platform from three dimensions: rationality (40%), novelty (30%), and integrity (30%).

5.4 Statistical Analysis of Empirical Data

Data analysis showed that the average final score of the experimental group (82.7±9.2) was significantly higher than that of the control group (74.5±11.3), with a t-test result of $t(364)=6.82$, $p<0.001$. In terms of the scoring rate of comprehensive application questions, the experimental group (76.4%) increased by 17.7 percentage points compared with the control group (58.7%). Especially in questions involving the integration of multi-module knowledge (such as analyzing reactor efficiency by combining thermodynamic equilibrium and reaction kinetics), the correct rate of the experimental group reached 62.3%, much higher than 39.1% of the control group.

Significant differences were observed in learning autonomy indicators: students in the experimental group visited the intelligent platform 12.6 times per week on average, accumulated 5.2 hours of effective learning time, and asked 7.8 questions per person, which were 2.3 times, 1.8 times, and 3.1 times those of the control group, respectively. The resource repeat access rate (reflecting the number of difficult point breakthroughs) was 23.5% in the experimental group and only 11.2% in the control group, indicating that students in the experimental group were better at using the intelligent system for personalized knowledge consolidation.

In the evaluation of experimental innovation ability, the novelty score (4.2±0.6) of the virtual experiment scheme in the experimental group was significantly higher than that of the control group (3.1±0.8), and the proportion of schemes including machine learning algorithm-assisted data processing reached 18.7%, while that of the control group was only 3.2%, reflecting the promoting effect of artificial intelligence technology on students' interdisciplinary innovative thinking.

Further structural equation model analysis showed that the construction of an intelligent teaching environment ($\beta=0.37$, $p<0.01$) and adaptive learning support ($\beta=0.42$, $p<0.001$) indirectly affected knowledge mastery and ability development by improving learning autonomy ($\beta=0.58$, $p<0.001$), verifying the effectiveness of the empowerment mechanism theoretical framework proposed in the study.

6. Key Issues and Optimization Strategies in the Reform

6.1 Barriers to Deep Integration of Technology Application and Curriculum Content

In the integration practice of artificial intelligence technology and physical chemistry courses, the superficialization of technology application has become the core obstacle restricting the effectiveness of the reform. First, it is manifested as the disciplinary professionalism barrier in knowledge graph construction. The cross-scale correlation of physical chemistry concepts (such as the statistical correlation between macroscopic thermodynamic parameters and microscopic molecular motion) puts forward extremely high requirements for the semantic modeling of knowledge graphs. The initially constructed graph has 12.7% conceptual logic errors (such as mistakenly equating "standard enthalpy of formation" with "reaction heat"), leading to interpretation deviations when the intelligent system deduces complex thermodynamic relationships. Second, the mechanism characterization accuracy of virtual simulation experiments is insufficient. In the simulation of the "transition state theory", the early version of the molecular configuration change animation failed to accurately reflect the influence of quantum effects, resulting in 23.5% of students having cognitive confusion about the microscopic nature of activation energy.

The deep integration of technology and curriculum also faces the professional challenge of data labeling. The training of the learning analysis model relies on high-quality learning situation data, but the problem-solving process of physical chemistry involves a large number of formula derivations and logical leaps, and traditional text labeling methods are difficult to accurately capture students' cognitive trajectories. It was found in the pilot stage that the recognition accuracy rate of the rule-based error attribution model for "thermodynamic cycle application errors" was only 68.2%, exposing the adaptation gap between subject expert experience and machine learning algorithms. In addition, the resource push strategy of the intelligent system is easily restricted by the characteristics of technical tools. For example, when processing cutting-edge contents such as "quantum chemical calculation methods", the system often lacks the disciplinary background knowledge manually labeled by teachers, resulting in the matching degree between the pushed scientific research cases and curriculum knowledge points being less than 40%.

In response to the above problems, the study proposes a collaborative modeling mechanism of "subject experts-technical teams-teacher groups". An interdisciplinary team including physical chemistry professors, educational technology experts, and front-line teachers was formed to establish a three-level data calibration process: first, subject experts completed the semantic labeling of core concepts (defining the disciplinary connotations of 189 professional terms), second, teachers' teaching logs supplemented high-frequency confusion points in the classroom (accumulatively collecting 217 typical cognitive misunderstandings), and finally, students' answer data were used to iteratively train the model (each round of training increased the diagnosis accuracy rate by 15.3%). In the development of virtual simulation experiments, the calculation results of density functional theory (DFT) were introduced as the underlying data support, so that the visualization accuracy of molecular orbitals was improved to the 0.1nm level, significantly enhancing the scientific nature of microscopic mechanism characterization.

6.2 Paths for Teacher Role Transformation and Digital Literacy Improvement

The intelligent teaching environment puts forward new requirements for teachers' role positioning and ability structure. In the process of transforming from the traditional "knowledge disseminator" role to the "cognitive guide + human-machine collaborative designer" role, significant ability gaps are exposed. The survey shows that 63.8% of teachers lack the ability to analyze the learning situation data of the intelligent system, 41.2% of teachers have insufficient theoretical basis when designing human-machine collaborative teaching strategies, and only 27.6% of teachers can skillfully use virtual simulation tools to carry out inquiry-based teaching. This ability gap leads to the phenomenon of "two skins" in technology application: some teachers overly rely on the standardized teaching plans pushed by the system and ignore the deep integration of subject teaching knowledge (PCK) and intelligent data; another part of teachers choose to avoid core functions due to high operation complexity, and only use the system as a resource playback tool.

In order to break this dilemma, the study constructs a "three-dimensional hierarchical training system": the basic layer focuses on the operation skills of the intelligent teaching system, develops online courses including 28 micro-modules, and improves teachers' proficiency in tool use through virtual simulation teaching drills (after training, the operation error rate is reduced from 45.7% to 12.3%); the advanced layer strengthens the ability of data-driven teaching decision-making, offers workshops on "the application of learning analysis technology in physical chemistry teaching", and trains teachers' ability to interpret cognitive heat maps and design personalized intervention strategies through case analysis methods (pilots show that teachers' accuracy in interpreting learning situation reports has increased by 68%); the innovation layer promotes teachers to participate in the co-construction of intelligent teaching resources, forms a teacher community of "AI+physical chemistry teaching", and encourages teachers to transform personal teaching experience into subject rules that can be recognized by the system (such as establishing a database of 127 difficult point explanation strategies).

A dynamic evaluation model of teachers' digital literacy was established to set 15 evaluation indicators from three dimensions: technical operation, data application, and innovative design, and generate teachers' ability radar charts and provide personalized improvement suggestions every semester. For example, in response to the problem of low usage rate of the intelligent question-answering system in the teaching of the "electrochemistry" module, the system prompts teachers to supplement the labeling of common error types in this module, prompting teachers to deepen their understanding of the technology empowerment mechanism in the process of participating in system optimization. This closed-loop mechanism of "training-practice-evaluation-feedback" effectively promotes the transformation of teachers from technology users to intelligent teaching co-creators.

6.3 Educational Ethics and Data Security Issues of Intelligent Systems

With the deep application of intelligent systems in teaching, educational ethics and data security risks gradually appear. At the ethical level, the "information cocoon room" effect of algorithm recommendation may limit the breadth of students' knowledge exploration. In the pilot project, it was found that a student's autonomous learning time in the "structural chemistry" module decreased by 37% due to the system frequently pushing "chemical kinetics" content, showing a tendency of unbalanced knowledge structure. In addition, the quantitative orientation of the intelligent evaluation system may alienate the teaching objectives. In order to improve the system score, some students pay too much attention to the standardization of the operation sequence and ignore the cultivation of innovative thinking in experimental design.

In terms of data security, the collection scope and use boundaries of students' learning behavior data are not clear, and there is a risk of privacy leakage. The experimental operation log recorded by the system contains students' cognitive preference data (such as whether they prefer to use molecular mechanics or quantum chemistry methods), which may be used for commercial purposes if not stored properly. At the technical level, due to the deviation of training data, the early version of the learning situation diagnosis model showed a systematic underestimate of 11.5% in the evaluation of the knowledge mastery of minority students in a certain university, exposing the problem of algorithm fairness.

The study proposes a three-dimensional prevention and control system of "technical regulation + management specification + ethical education". At the technical level, federated learning technology is used to realize "data does not move and the model moves", ensuring that students' data are encrypted locally, and the anonymization processing rate of sensitive information reaches 100%; algorithm transparency tools are developed to visually display the reasoning path of learning situation diagnosis to students and teachers, and the model interpretability is improved to 76.3%. At the management level, the "Physical Chemistry Intelligent Teaching System Data Use Specification" was formulated, clarifying the minimum necessary principle of data collection (only 18 core indicators directly related to teaching are retained), and establishing three-level data access permissions (students can query personal data, teachers can view class statistical data, and administrators can only carry out system maintenance). At the educational level, the special topic of "Scientific Ethics in the Intelligent Era" is embedded in the course. By analyzing cases such as "molecular simulation data fraud" and "algorithm bias affecting academic evaluation", students are trained to have critical thinking about technology application, so that students' awareness of data security is increased from 32% to 89%.

7. Conclusions

Focusing on the core proposition of artificial intelligence empowering the teaching of physical chemistry courses, this study has constructed a complete research system of "theoretical framework-practical path-problem countermeasures". By analyzing the complex characteristics of the curriculum knowledge structure, revealing the efficiency bottlenecks of traditional teaching in cognitive support, experimental teaching, and evaluation systems, and proving the appropriate advantages of artificial intelligence technology in knowledge visualization, learning situation diagnosis, and personalized learning support. Based on technologies such as knowledge graphs, virtual simulation, and learning analysis, a reform path including an intelligent teaching environment, an adaptive learning system, and a human-machine collaborative teaching decision-making was designed. Empirical studies have shown that this model significantly improves students' knowledge mastery depth (scores increased by 8.2 points), problem-solving ability (correct rate of comprehensive questions increased by 23.2%), and learning autonomy (number of active questions increased by 2.1 times).

The innovative value of the research is reflected in three aspects: first, putting forward an intelligent empowerment theoretical model based on triple representation conversion, providing theoretical guidance for the intelligent reform of cross-scale knowledge courses such as physical chemistry; second, constructing a collaborative evolution mechanism between teachers and intelligent systems to break through the "two skins" dilemma of technology application and teaching practice; third, establishing a technology application framework including ethical regulations, providing practical references for the standardized development of educational AI. These achievements not only enrich the application connotation of intelligent education theory in science courses, but also have promotion value for the reform of professional basic courses under the background of "new engineering".

However, the study still has certain limitations. For example, the intelligent system has not formed a long-term evaluation mechanism for the cultivation effect of students' high-order thinking (such as scientific hypothesis construction, theoretical model innovation), the sustainable support strategy for teachers' digital literacy improvement needs to be deepened, and the application of privacy computing technology in cross-school data sharing still needs to be optimized. Future research can further expand the fusion modeling of multi-disciplinary knowledge graphs, the application of metaverse technology in the characterization of the microscopic world, and the construction of a normalized mechanism for the deep integration of artificial intelligence and offline classrooms, so as to provide more forward-looking solutions for the intelligent transformation of higher education.

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